Registry Number:

122320-73-4

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Formula:

C18 H19 N3 O3 S

CA Index Name:

2,4-Thiazolidinedione, 5-[[4-[2-(methyl-2-pyridinylamino)ethoxy]phenyl]methyl]- (9CI)

Other Names:

5-[4-[2-(N-Methyl-N-(2-pyridyl)amino)ethoxy]benzyl]thiazolidine-2,4-

dione; BRL 49653; Rosiglitazone

-- Properties --

| | Calculated | | |
|------------------|------------------|------------------|-------------|
| <u>Property</u> | <u>Value</u> | Condition | <u>Note</u> |
| Bioconc. Factor | 1 | pH 1 | (1) ACD |
| Bioconc. Factor | 1 | pH 4 | (1) ACD |
| Bioconc. Factor | 7.30 | pH 7 | (1) ACD |
| Bioconc. Factor | 1.11 | pH 8 | (1) ACD |
| Bioconc. Factor | 1 | pH 10 | (1) ACD |
| Boiling Point | 585.0±35.0 °C | Press: 760.0 | (1) ACD |
| | | Torr | |
| Enthalpy of Vap. | 87.40±3.0 kJ/mol | | (1) ACD |
| Flash Point | 307.6±46.7 °C | | (1) ACD |
| H acceptors | 6 | | (1) ACD |
| H donors | 1 | | (1) ACD |
| Koc | 1 . | pH 1 | (1) ACD |

| Koc | 2.03 | pH 4 | (1) ACD |
|------------------|-------------------|---------------|----------------------|
| Koc | 82.7 | pH 7 | (1) ACD |
| Koc | 12.5 | pH 8 | (1) ACD |
| Koc | 1 | pH 10 | (1) ACD |
| logD | -1.43 | pH 1 | (1) ACD ⁻ |
| logD | 0.10 | pH 4 | (1) ACD |
| logD | 1.71 | pH 7 | (1) ACD |
| logD | 0.89 | pH 8 | (1) ACD |
| logD | -0.96 | pH 10 | (1) ACD |
| logP | 2.560±0.785 | | (1) ACD |
| Molar Solubility | Soluble | pH 1 | (1) ACD |
| Molar Solubility | Slightly Soluble | pH 4 | (1) ACD |
| Molar Solubility | Sparingly Soluble | рH 7 | (1) ACD |
| Molar Solubility | Sparingly Soluble | pH 8 | (1) ACD |
| Molar Solubility | Soluble | pH 10 | (1) ACD |
| Molecular Weight | 357.43 | | (1) ACD |
| рКа | 6.34±0.50 | Most Acidic | (1) ACD |
| рКа | 6.48±0.12 | Most Basic | (1) ACD |
| Vapor Pressure | 1.14E-13 Torr | Temp: 25.0 °C | (1) ACD |

Notes:

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 (© 1994-2004 ACD)

-- Resources --

References:

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STN Files:

CAPLUS, ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR,

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